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Practical elastic photon-scattering calculations: available data and on-line access via the World Wide Web

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Abstract: Using state-of-the-art S-matrix predictions to characterize the angular dependence of the anomalous-scattering-factor approximation, it now appears likely that practical, accurate predictions of elastic photon-atom scattering should be achievable for all $Z = 1 - 99$, all $\hbar\omega = 0 - 10$ MeV. New S-matrix calculations for all Z on a 56-point energy grid are being prepared to support this effort.
The availability of elastic-scattering information on the World Wide Web is reviewed.

Keywords: elastic photon-atom scattering, Rayleigh scattering, form factors, anomalous scattering factors

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1. Introduction

A variety of important applications require accurate elastic photon-atom scattering predictions beyond that readily available today. While the S-matrix approach (see, for example, Ref. [1-21]) has yielded accurate prognostications in many cases of experimental and theoretical interest, the method has not yet yielded predictions that are easily obtained for all cases of practical interest. In order to correct this inadequacy, a serious computational effort is

underway to create a dense grid of S-matrix benchmark data that will support extension to all Z and all $\hbar\omega$ of interest.

Because of the rich energy structure in the elastic-scattering process for photon energies in the x-ray regime, direct interpolation on S-matrix predictions is impractical except for limited energy regions away from atomic thresholds. Fortunately, through careful inclusion of important contributions that have been historically neglected, anomalous scattering factors have been found to reproduce the forward-angle S-matrix scattering amplitude [4] to a very high degree of accuracy. In fact, the difference between complete anomalous-scattering-factor predictions and forward-angle S-matrix results are generally at the limit of accuracy of the numerical calculations that have been performed (of the order of a fraction of a percent in most cases).

However, there is no theory for the angular dependence of anomalous-scattering-factor predictions that yield the same good agreement with S-matrix results for non-forward angles at all Z and energies of interest. By using of the S-matrix approach to characterize the angular dependence of the anomalous-scattering-factor approximation, it now seems likely that practical, accurate elastic-scattering predictions for all photon energies of interest, for all atoms in the periodic table and all scattering angles should now be realizable. The extension to scattering from ions, excited or hollow atoms should be straight forward.

2. Scattering Formalism

Our formalism for elastic photon scattering from isolated atoms or ions has been adequately described elsewhere (see, for example, Ref. [1-4]). The expressions shown here will largely be only those needed to support the discussions that follow.

The scattering of photons by atoms is assumed to be adequately described by the second-order S-matrix amplitude as

$$A = -\sum_P \left[\frac{\langle N|O_f^*|P\rangle\langle P|O_i|N\rangle}{E_N - E_P + \hbar\omega + i0_+} + \frac{\langle N|O_i|P\rangle\langle P|O_f^*|N\rangle}{E_N - E_P - \hbar\omega - i0_+} \right], \tag{1}$$

The elastic-scattering cross section is computed as

$$\frac{d\sigma}{d\Omega} = |A|^2, \tag{2}$$

where $\hbar\omega$ is the energy of the incident (or scattered) photon, the operator O_i (O_f^*) describes the absorption (emission) of the incident (scattered) photon, $i = \sqrt{-1}$, 0_+ is a small positive value, and the states $|N\rangle$ and $|P\rangle$ are properly symmetrized solutions of the many-particle Dirac equation for noninteracting particles.

It is traditional to partition the amplitudes for scattering off an atomic system into amplitudes for scattering off its components, and call these the component amplitudes for Rayleigh (R), nuclear Thomson (T), and Delbrück (D) scattering (to be added coherently, since they cannot be distinguished in any observation):

$$A = A^{\mathrm{R}} + A^{\mathrm{T}} + A^{\mathrm{D}}. \tag{3}$$

Pratt et al. [3] present a more detailed discussion of this partitioning and the steps needed to reduce the many-particle scattering problem to a single-particle description of scattering.

To lowest order in the fine structure constant, the optical theorem for Rayleigh scattering states that

$$\mathrm{Im}A^{\mathrm{R}}(\omega, 0) = \frac{\omega}{4\pi c}(\sigma^{\mathrm{PE}} + \sigma^{\mathrm{BBT+}} - \sigma^{\mathrm{BBT-}} - \sigma^{\mathrm{BPP}}) \tag{4}$$

where σ^{PE} is the cross section for photoeffect, $\sigma^{\mathrm{BBT+}}$ is the cross section for a transition from the initial state to a excited bound state of the system, $\sigma^{\mathrm{BBT-}}$ is the cross section for a transition from the initial state to a bound state of lower energy, and σ^{BPP} is the cross section for bound-electron pair production. The bound-bound contributions are computed as

$$\sigma^{\mathrm{BBT+}}(\omega) = \frac{2\pi^2 c r_0}{\omega} \sum_{n,\, m>n} \omega_{nm} f_{nm} \delta(\omega - \omega_{nm}), \tag{5}$$

and

$$\sigma^{\mathrm{BBT-}}(\omega) = \frac{2\pi^2 c r_0}{\omega} \sum_{n,\, m<n} \omega_{nm} f_{nm} \delta(\omega - \omega_{nm}), \tag{6}$$

where f_{nm} is the oscillator strength for the transition of energy $\hbar\omega_{nm}$ of an

electron from occupied state n to unoccupied state m. (The notation $m > n$ / $m < n$ indicates the sum over unoccupied states m with energies less than / greater than the occupied state n. For ground-state atoms, the contribution from Eq. (6) is zero.) Although the total cross section at x-ray energies is dominated by absorption, primarily atomic photoeffect, contributions from bound-bound transitions (see, for example, Wang & Pratt [5]) must be included if accurate results are to be obtained from the dispersion relation for low-energy scattering.

General considerations of rotational invariance and parity conservation allow the Rayleigh scattering amplitude for scattering of an incident photon of momentum $\boldsymbol{k}_i$ and polarization $\boldsymbol{\varepsilon}_i$, elastically scattered to a state of momentum $\boldsymbol{k}_f$ and polarization $\bar{\boldsymbol{\varepsilon}}_f$ to be written in the form

$$A^{\mathrm{R}} = (\boldsymbol{\varepsilon}_i \bullet \boldsymbol{\varepsilon}_f^*)\, \mathcal{M}(\boldsymbol{k}_i \bullet \boldsymbol{k}_f) + (\boldsymbol{\varepsilon}_i \bullet \boldsymbol{k}_f)\, (\boldsymbol{\varepsilon}_f^* \bullet \boldsymbol{k}_i)\, \mathcal{N}(\boldsymbol{k}_i \bullet \boldsymbol{k}_f)\,, \qquad (7)$$

where $\mathcal{M}$ and $\mathcal{N}$ are complex functions of the scattering angle (they only depend on the inner product $\boldsymbol{k}_i \bullet \boldsymbol{k}_f$), and the atom has been assumed to be rotationally invariant (i. e., composed of filled subshells). For atoms with open subshells, additional amplitudes would need to be considered. Some researchers (see, for example, Ref. [22,23]) have used tensors to describe scattering effects such as dichronism, birefringence, and anisotropic dispersion; effects beyond those given by Eq. (7).

Note that only the first term in Eq. (7) contributes for forward-angle scattering or in dipole or form-factor approximations; through the x-ray regime it varies relatively slowly with energy.

If we decompose the polarization vector into components parallel and perpendicular to the scattering plane (defined by vectors $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$),

$$\boldsymbol{\varepsilon}_i = \varepsilon_i^{\parallel}\hat{\boldsymbol{\varepsilon}}_i^{\parallel} + \varepsilon_i^{\perp}\hat{\boldsymbol{\varepsilon}}_i^{\perp}\,, \quad \boldsymbol{\varepsilon}_f = \varepsilon_f^{\parallel}\hat{\boldsymbol{\varepsilon}}_f^{\parallel} + \varepsilon_f^{\perp}\hat{\boldsymbol{\varepsilon}}_f^{\perp}\,, \qquad (8)$$

it is easy to show that

$$A^{\mathrm{R}} = \varepsilon_i^{\parallel}\varepsilon_f^{\parallel}A_{\parallel}^{\mathrm{R}} + \varepsilon_i^{\perp}\varepsilon_f^{\perp}A_{\perp}^{\mathrm{R}}\,, \qquad (9)$$

where

$$A_{\parallel}^{\mathrm{R}} = \mathcal{M}\cos\theta - \mathcal{N}\sin^2\theta\,, \; A_{\perp}^{\mathrm{R}} = \mathcal{M}. \qquad (10)$$

(In this notation, $\boldsymbol{\varepsilon}_i$ is the polarization of the incident photon, $\hat{\boldsymbol{\varepsilon}}_i^{\parallel}$ is a unit vector that is parallel to the plane of scattering and perpendicular to $\boldsymbol{k}_i$, while $\hat{\boldsymbol{\varepsilon}}_i^{\perp}$ is a unit vector that is perpendicular to the plane of scattering and perpendicular to $\boldsymbol{k}_i$.) The scattering angle θ is the angle between $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ ($\theta = 2\Theta$, where Θ is the Bragg angle). The cross section for scattering of initially unpolarized photons where the polarization of the scattered photon is not observed is obtained by averaging over incident photon polarizations and summing over scattered photon polarizations:

$$\frac{d\sigma}{d\Omega} = \frac{1}{2}\left(\left|A_{\parallel}^{R}\right|^2 + \left|A_{\perp}^{R}\right|^2\right) . \tag{11}$$

The general case of polarized scattering is discussed by Roy et al. [6] in terms of Stokes parameters.

3. New S-Matrix Calculations

S-matrix Rayleigh-scattering calculations have been performed by Brown and co-workers [7-9], Johnson and co-workers [10-12], and Kissel & Pratt and co-workers [1-4,13-18]. Until now, the most extensive published tabulation of S-matrix results was given by Kane et al. [2] wherein values for 10 elements $Z = 13 - 103$, for 7 energies $\hbar\omega = 60 - 1332$ keV, at 55 angles $\theta = 0 - 180°$ were presented. S-matrix predictions have been found to generally agree with experiment to within several percent as long as the photon energy is not too near to atomic thresholds.

Our general prescription involves explicit calculation of the S-matrix amplitude for inner-shell electrons (which we have traditionally defined as electrons with photon-energy to binding-energy ratios $\hbar\omega/\varepsilon \leq 300$), combined with estimates for outer-shell electrons computed from modified relativistic form factors [1]. Nearer to atomic thresholds, energy scaling procedures have been found to improve the predictions [17, 19, 20].

Another recent improvement in our method involves an explicit subtraction of spurious bound-bound resonance contributions (contributions from bound-bound transitions between occupied orbitals) from the inner-electron S-matrix amplitudes [20]. Our current implementation involves the subtraction of the spurious resonance "after the fact" -- a numerical subtraction of the resonant contributions from the numerical S-matrix amplitude which includes the resonances. This procedure will increasingly fail as one approaches a spurious resonance, due to catastrophic lose of precision. A better solution, not yet implemented, would be a "before the fact" subtraction --

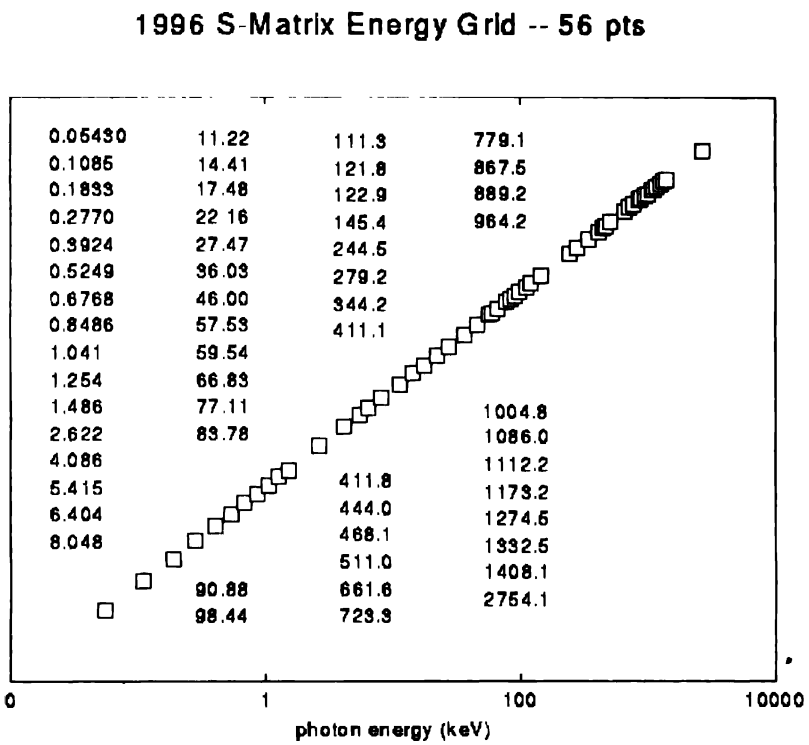

Fig. 1. The photon energies (in keV) are listed and graphically depicted for the new systematic tabulation of elastic-scattering cross sections and amplitudes.

an analytic subtraction of the spurious resonance from the differential equations that are solved to compute the scattering amplitude.

Although S-matrix calculations are numerically intensive, advances in computing technology and improvements to the computer programs used in this calculation have made much more extensive calculations feasible. To support the systematic generation of all $Z = 1-99$, all $\hbar\omega = 0-10$ MeV state-of-the-art elastic-scattering tables, new S-matrix calculations are being completed. Explicit calculations on a uniform 56-point energy grid (see Fig. 1.) are being computed for all subshells wherein photon energy to electron binding ratio $\hbar\omega/\varepsilon \leq 1000$. These values represent a significant expansion over the data that has been formerly available, with the extension of the calculation to all atoms being the most significant. Tables of unpolarized scattering cross sections and linearly-polarized scattering amplitudes are being prepared on a single non-uniform 97-point angle grid (i.e., the same angle grid is used in all cases, but the grid is not uniform in angle, being denser at small

angles). The angle grid used is an expanded version of our 55-point grid [2] that yields interpolated $\theta, \log(d\sigma/d\Omega)$ results accurate to about 1%. In total, differential S-matrix scattering predictions are being tabulated at over 1/2 million individual $(Z, \hbar\omega, \theta)$ points. Twenty-six (26) individual 40 to 60-MHz SPARC CPUs (mostly Sun SPARCstation model 10 workstations) are being utilized in parallel to prepare these tables for an integrated effort of about 1.5 CPU years. Some sample predictions are shown in Fig. 2.

In spite of this significant application of modern computing technology to the problem of elastic scattering, it is evident from the inspection of Fig. 2. that direct interpolation on the differential cross section will not yield satisfactory predictions throughout our energy region of interest, especially for photon energies near atomic binding energies. But, it has been shown that modified relativistic form factors (MF) with angle-independent anomalous scattering factors (ASF) provide accurate predictions compared with SM values for forward angles [4]. So it would seem reasonable that SM/MF+ASF ratios will provide a basis for interpolation to intermediate energies.

4. MF+ASF Approximation

In a generalization of the usual anomalous-scattering-factor approximation for elastic scattering, we write

$$\mathcal{M}(\omega, \theta) = -r_0 [f(q) + f'(\omega, \theta) + if''(\omega, \theta)], \tag{12}$$

or

$$\mathcal{M}(\omega, \theta) = -r_0 [g(q) + g'(\omega, \theta) + if''(\omega, \theta)], \tag{13}$$

and

$$\mathcal{N}(\omega, \theta) = -r_0 [f'''(\omega, \theta) + if''''(\omega, \theta)]. \tag{14}$$

We call the real quantities g' or f', f'', f''', f'''' *anomalous scattering factors*. As they are defined here, these factors give the deviation of the total angle-dependent scattering amplitude from the amplitude predicted by the form-factor approximation.

We choose to utilize anomalous scattering factors defined relative to the modified relativistic form factor (MF) $g(q)$, rather than the form factor (FF) $f(q)$, as the MF has been shown numerically to have nearly the correct high-

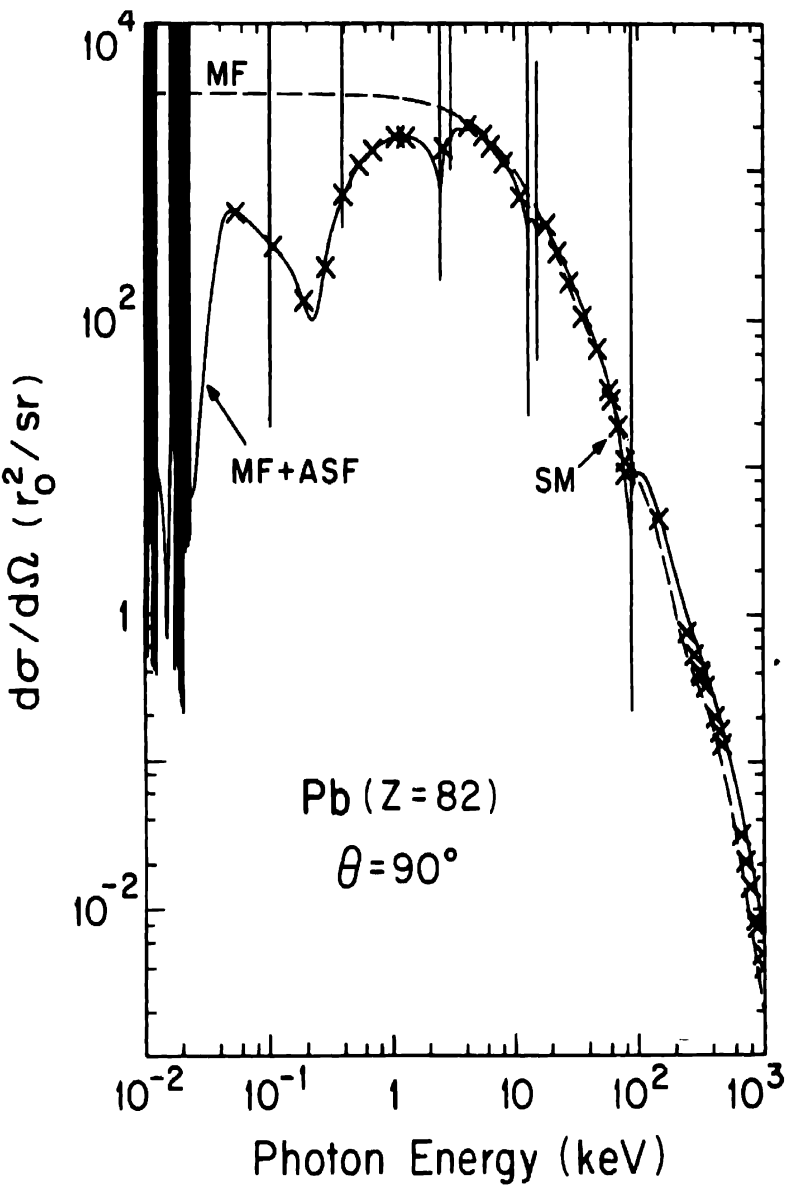

Fig. 2. Differential cross sections of Rayleigh scattering in various approximations for lead for $\theta = 90°$. The crosses represent explicit S-matrix (SM) predictions, shown with modified-relativistic-form-factor (MF) and angle-independent anomalous-scattering-factor (MF+ASF) predictions.

energy limit in the forward direction. Consequently, the corresponding real correction $g'(\infty, 0) \approx 0$, whereas $f'(\infty, 0) \approx N - g(0)$ is finite. The total-atom modified form factor is given as

$$g(q) = \sum_n g_n(q) = 4\pi \sum_n \int_0^\infty \rho_n(r) \frac{\sin qr}{qr} \left[\frac{mc^2}{E_n - V(r)} \right] r^2 dr . \tag{15}$$

A complete tabulation of MF values can be found in Schaupp et al. [25], in which $g(q)$ for all elements in the periodic table were calculated using relativistic wavefunctions and potentials (total-atom and K-shell MF values are listed).

The forward-angle values of g' or f', f'', but not f''', f'''', can be computed from the dispersion relations

$$\mathrm{Re}A(\omega, 0) = \frac{2\omega^2}{\pi} \int_0^\infty \frac{\mathrm{Im}A(\omega', 0)}{\omega' (\omega'^2 - \omega^2)} d\omega' , \tag{16}$$

$$\mathrm{Im}A(\omega, 0) = -\frac{2\omega}{\pi} \int \frac{\mathrm{Re}A(\omega', 0)}{\omega'^2 - \omega^2} d\omega' , \tag{17}$$

so that

$$\mathrm{Re}A(\infty, 0) = -\frac{2}{\pi} \int \frac{\mathrm{Im}A(\omega', 0)}{\omega'} d\omega' \quad , \quad \mathrm{Im}A(\infty, 0) = 0 . \tag{18}$$

Or

$$f'(\omega, 0) = g'(\omega, 0) - \left(N + \frac{\mathrm{Re}A^R(\infty, 0)}{r_0} \right) \tag{19}$$

where

$$g'(\omega, 0) = \frac{2}{\pi} \int^{\infty} \frac{\omega' f''(\omega', 0)}{\omega'^2 - \omega^2} d\omega', \tag{20}$$

and by Eq. 4,

$$f''(\omega, 0) = -\frac{\omega}{4\pi c r_0} \tau^{TOT} \tag{21}$$

It should be noted that the sign of our f'' differs from that commonly given in the crystallographic literature, f''_{CL} or f_2^{Henke} (see, for example, Cromer [26]; Creagh and McAuley [27]; Henke et al. [28]) as

$$f''_{CL} = f_2^{Henke} = -f''. \tag{22}$$

This difference has its origins in a sign choice for the plane wave. This issue has been discussed by Ramaseshan et al. [29] who pointed out problems comparing neutron and x-ray scattering where differing phase conventions are used.

5. SM/(MF+ASF) Ratios as a Basis for Interpolation in Photon Energy

Sample SM/(MF+ASF) ratios of the unpolarized differential cross section have been prepared; data for $_{82}$Pb are shown in Fig. 3. Each curve in this figure represents the differential cross-section ratio at a fixed scattering angle.

As expected, the ratio for forward-angle scattering is very close to one. It is also seen that the accuracy of the angle-independent anomalous-scattering-factor approximation decreases with increasing angles at higher energies; MF+ASF predictions are too large by about a factor of 5 for 60° scattering around 1 MeV.

The data for lead was selected for this example because the errors in MF+ASF predictions at finite angle are largest for high-Z atoms. A similar comparison for a light-Z atom such as carbon would show remarkably little difference between SM and MF+ASF predictions for all energies and angles.

In spite of the errors in MF+ASF predictions of up to a factor of five shown in Fig. 3, we see that the MF+ASF approximation has done a fantastic job in smoothing the variation in the SM predictions. If we look again at Fig. 2, which shows the differential cross section for 90° scattering by lead (a

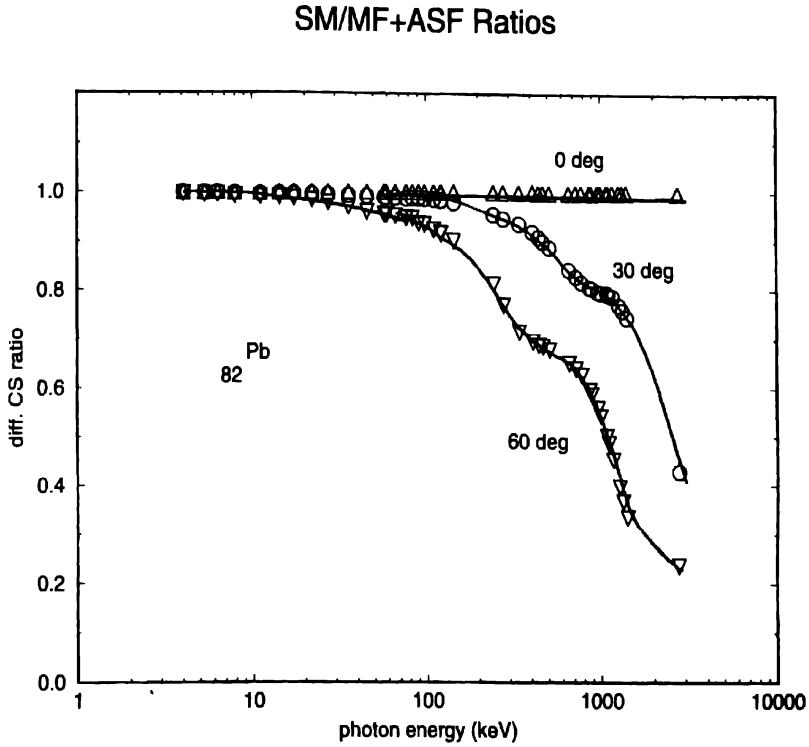

Fig. 3. SM/(MF+ASF) ratios for the unpolarized differential cross section, for lead.

plot for 60° scattering would look very similar), we see that the cross section has changed by over 5 orders of magnitude through 100-1000 keV, yet the cross-section ratio has only changed by a factor of 5! Even more remarkably, the narrow, "spiky" bound-bound resonances shown in the cross sections of Fig. 2 have been completely removed in the ratios of Fig. 3.

We are currently investigating two somewhat different approaches for interpolating on the benchmark SM data: a "direct" approach following the ideas suggested in Fig. 3; and a more indirect approach based on a characterization of the angular dependence of the anomalous scattering factors.

Fig. 3 suggests that a direct fit to SM/(MF+ASF) ratios should be possible. However, it is anticipated that this direct approach will prove to be unwieldy. For example, individual fits to curves like those shown in Fig. 3 could result in 97 separate fits (one for each of the 97 angles in our benchmark grid) for each atom. Assuming that we would be able to characterize these curves with as few as 5 parameters each, on the average, this would result in

a table of about 50,000 parameters. If we wanted to characterize polarized amplitudes (needed for many applications) instead the unpolarized cross section, we might need upwards of $4 \times 50{,}000 = 200{,}000$ parameters!

An alternate approach we are investigating takes a lead from the form of nonrelativistic Coulomb K-shell ASF angular distribution derived by Costescu et al. [24]. We anticipate that fits to the angular distribution of the anomalous scattering factors are possible using a form similar to:

$$f^{(i)}(\omega, \theta) = f^{(i)}(\omega, 0)\left[a_0^{(i)} + a_1^{(i)} \sin^2\frac{\theta}{2} + a_2^{(i)} \sin^4\frac{\theta}{2} + \ldots\right]. \quad (23)$$

where $f^{(i)}$ indicates one of f', f'', f''', f''''. Since the forward-angle values of f', f'' are available to us from the dispersion integral and optical theorem, Eq. (18) through Eq. (21), we set

$$a_0' \equiv a_0'' \equiv 1. \quad (24)$$

Since we do not have an comparable knowledge of the forward-angle values of f''', f'''', we must evaluate the constant term of these expansions from the fit.

The coefficients $a_k^{(i)}$ are a function of $\hbar\omega$ and Z, but independent of θ. It is anticipated that curves for the $a_k^{(i)}$ similar to those shown in Fig. 3 will be obtained. Assuming that 5 terms will be needed, on the average, in the series of Eq. (23), and that each $a_k^{(i)}$ curve for variable $\hbar\omega$ and fixed Z will need a 5-parameter fit, the resulting benchmark table would contain $5 \times 5 \times 100 = 2500$ parameters. If successful, this indirect approach would provide polarized amplitudes, and consequently both polarized and unpolarized cross sections.

6. On-Line Data Available on the World Wide Web

The world is experiencing an explosive growth in electronic communications which dramatically reduces the distance that separates individuals who have access to this *cyberspace*. An exciting component of this new dimension of the human intellect is the Internet and particularly the World Wide Web. Soon every student in the US, from grade school through graduate school, will have ready access to this medium. All countries of the world are rapidly expanding their connections to *the Web*. Already a significant amount of scientific data is on-line and accessible from most places on the planet.

In what follows, we briefly mention some sites offering information of

interest to the x-ray and radiation-physics community. Be warned though, the Web is a living document; it is constantly changing, with additions and deletions taking place daily -- which is both a strength and a weakness..

Elastic Photon-Atom Scattering – Kissel/Bergstrom – LLNL

We are making our elastic-scattering data available on-line. It is accessible at the URL (Universal Resource Locator)

http://www-phys.llnl.gov/V_Div/scattering/elastic.html

Our data files are also available via anonymous ftp at the URL

ftp://www-phys.llnl.gov/rayleigh

After reaching our site, one can obtain:

- S-matrix amplitudes and cross sections,
- unpolarized and polarized, differential and total elastic scattering cross sections in NF, RF, MF, RF+ASF, MF+ASF approximations;
- our anomalous scattering factors;
- nonrelativistic, relativistic, and modified relativistic form factors;
- angular dependence of anomalous scattering factors based on nonrelativistic Coulomb K-shell results.

X-Ray Interactions with Matter – Gullikson/Henke – LBL

The work of Henke et al. [28], is available from Lawrence Berkeley Laboratory at URL

http://www-cxro.lbl.gov/

At this site you can access:

- anomalous scattering factors f_1, f_2 based on a synthesis of experimental and theoretical data;
- x-ray properties of the elements and simple mixtures;
- predicted response functions of x-ray optical components including filter transmission, mirror reflectivity, reflectivity of synthetic multilayers, diffraction efficiency of transmission gratings;
- pointers to other WWW sites.

X-Ray WWW Server – Uppsala University

This was one of the earliest Web sites with x-ray data. It is accessible at

http://xray.uu.se/

Started in April, 1994, this site offers:

- Henke et al. [28] anomalous scattering factors;
- Gwyn Williams' (Brookhaven National Laboratory, see, for example, Ref. [30]) experimental binding energies;
- J. A. Bearden's [31] K- and L-shell x-ray emission lines;
- oscillator strengths;
- pointers to other sites on the Web.

X-Ray Properties of the Elements

The Center for Synchrotron Radiation Research and Instrumentation supports a "clickable" periodic table with x-ray properties of the elements, accessible at the URL

http://www.csrri.iit.edu/periodic-table.html

"YAHOO!" x-ray physics pointers

Consult one of the more famous of the "search-engine" Web sites for pointers to other sites of interest at the URL

http://www.yahoo.com/Science/Physics/X_Ray/

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